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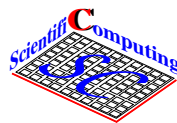
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Inverse problems and uncertainty quantification*

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Abstract

In a Bayesian setting, inverse problems and uncertainty quantification (UQ)—the propagation of uncertainty through a computational (forward) model—are strongly connected. In the form of conditional expectation the Bayesian update becomes computationally attractive. This is especially the case as together with a functional or spectral approach for the forward UQ there is no need for time-consuming and slowly convergent Monte Carlo sampling. The developed sampling-free non-linear Bayesian update is derived from the variational problem associated with conditional expectation. This formulation in general calls for further discretisation to make the computation possible, and we choose a polynomial approximation. After giving details on the actual computation in the framework of functional or spectral approximations, we demonstrate the workings of the algorithm on a number of examples of increasing complexity. At last, we compare the linear and quadratic Bayesian update on the small but taxing example of the chaotic Lorenz 84 model, where we experiment with the influence of different observation or measurement operators on the update.

Keywords: inverse problem, identification, uncertainty quantification

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1 Introduction

In trying to predict the behaviour of physical systems, one is often confronted with the fact that although one has a mathematical model of the system which carries some confidence as to its fidelity, some quantities which characterise the system may only be incompletely known, or in other words they are uncertain. See [23] for a synopsis on our approach to such parametric problems.

We want to identify these parameters through observations or measurement of the response of the system, which can be approached in different ways. In the mathematical description, the measurement / observation / output is determined by the uncertain parameters, i.e. we have a mapping from parameters to observations. The problem is that usually this mapping is not invertible, hence these inverse identification problems are generally ill-posed.

One way to deal with this difficulty is to measure the difference between observed and predicted system output and try to find parameters such that this difference is minimised. Frequently it may happen that the parameters which realise the minimum are not unique. In case one wants a unique parameter, a choice has to be made, usually by demanding additionally that some norm or similar functional of the parameters is small as well, i.e. some regularity is enforced. This optimisation approach hence leads to regularisation procedures [3].

Here we take the view that our lack of knowledge or uncertainty of the actual value of the parameters can be described in a *Bayesian* way through a probabilistic model [14, 36, 35]. The unknown parameter is then modelled as a random variable (RV)—also called the *prior* model—and additional information on the system through measurement or observation changes the probabilistic description to the so-called *posterior* model. The second approach is thus a method to update the probabilistic description in such a way as to take account of the additional information, and the updated probabilistic description *is* the parameter estimate, including a probabilistic description of the remaining uncertainty.

It is well-known that such a Bayesian update is in fact closely related to *conditional expectation* [2, 9], and this will be the basis of the method presented. For these and other probabilistic notions see for example [27] and the references therein. As the Bayesian update may be numerically very demanding, we show computational procedures to accelerate this update through methods based on *functional approximation* or *spectral representation* of stochastic problems [21]. These approximations are in the simplest case known as Wiener's so-called *homogeneous* or *polynomial chaos* expansion

[37], which are polynomials in independent Gaussian RVs—the ‘chaos’—and which can also be used numerically in a Galerkin procedure [8, 22, 21]. This approach has been generalised to other types of RVs [38]. It is a computational variant of *white noise analysis*, which means analysis in terms of independent RVs, hence the term ‘white noise’ [12, 13, 11], see also [22, 28], and [6] for here relevant results on stochastic regularity. Here we describe computational extensions of this approach to the inverse problem of Bayesian updating, see also [25, 31, 26, 29].

To be more specific, let us consider the following situation: we are investigating some physical system which is modelled by an evolution equation for its state:

$$\frac{\partial}{\partial t}u(t) + A(q; u(t)) = f(q; t), \quad (1)$$

where $u(t) \in \mathcal{U}$ describes the state of the system at time $t \in [0, T]$ lying in a Hilbert space \mathcal{U} (for the sake of simplicity), A is a—possibly non-linear—operator modelling the physics of the system, and $f \in \mathcal{U}^*$ is some external influence (action / excitation / loading). The model depends on some parameters $q \in \mathcal{Q}$ which are uncertain and which we would thus like to identify. To have a concrete example of Eq. (1), consider the diffusion equation

$$\frac{\partial}{\partial t}u(x, t) - \operatorname{div}(\kappa(x)\nabla u(x, t)) = f(x, t), \quad x \in \mathcal{G}, \quad (2)$$

with appropriate boundary and initial conditions, where $\mathcal{G} \subset \mathbb{R}^n$ is a suitable domain. The diffusing quantity is $u(x, t)$ (heat, concentration) and the term $f(x, t)$ models sinks and sources. Similar examples will be used for the numerical experiments in Section 4 and Section 5. Here $\mathcal{U} = H_E^1(\mathcal{G})$, the subspace of the Sobolev space $H^1(\mathcal{G})$ satisfying the essential boundary conditions, and we assume that the diffusion coefficient $\kappa(x)$ is uncertain. The parameters could be the positive diffusion coefficient field $\kappa(x)$, but for reasons to be explained fully later we prefer to take $q(x) = \log(\kappa(x))$, and assume $q \in \mathcal{Q} = L_2(\mathcal{G})$.

Our main application focus are models described by partial differential equations (PDEs) like Eq. (2), and discretised for example by finite element procedures. The updating methods have to be well defined and stable in a continuous setting, as otherwise one can not guarantee numerical stability with respect to the PDE discretisation refinement, see [35] for a discussion of related questions. Due to this we describe the update before any possible discretisation in the simplest Hilbert space setting. On the other hand no harm will result for the basic understanding if the reader wants to view the occurring spaces as finite dimensional Euclidean spaces.

Now assume that we observe a function of the state $Y(u(q), q)$, and from this observation we would like to identify the corresponding q . In the concrete example Eq. (2) this could be the value of $u(x_j, t)$ at some points $x_j \in \mathcal{G}$. This is called the *inverse* problem, and as the mapping $q \mapsto Y(q)$ is usually not invertible, the inverse problem is *ill-posed*. Embedding this problem of finding the best q in a larger class by modelling our knowledge about it with the help of probability theory, then in a Bayesian manner the task becomes to estimate conditional expectations, e.g. see [14, 36, 35] and the references therein. The problem now is *well-posed*, but at the price of ‘only’ obtaining probability distributions on the possible values of q , which now is modelled as a \mathcal{Q} -valued random variable (RV). On the other hand one naturally also obtains information about the remaining uncertainty. Predicting what the measurement $Y(q)$ should be from some assumed q is computing the *forward* problem. The *inverse* problem is then approached by comparing the forecast from the forward problem with the actual information.

Since the parameters of the model to be estimated are uncertain, all relevant information may be obtained via their stochastic description. In order to extract information from the posterior, most estimates take the form of expectations w.r.t. the posterior. These expectations—mathematically integrals, numerically to be evaluated by some quadrature rule—may be computed via asymptotic, deterministic, or sampling methods. In our review of current work we follow our recent publications [25, 31, 26, 29].

One often used technique is a Markov chain Monte Carlo (MCMC) method [18, 7], constructed such that the asymptotic distribution of the Markov chain is the Bayesian posterior distribution; for further information see [29] and the references therein.

These approaches require a large number of samples in order to obtain satisfactory results. Here the main idea here is to perform the Bayesian update directly on the polynomial chaos expansion (PCE) without any sampling [25, 31, 23, 26, 29]. This idea has appeared independently in [1] in a simpler context, whereas in [33] it appears as a variant of the Kalman filter (e.g. [15]). A PCE for a push-forward of the posterior measure is constructed in [24].

From this short overview it becomes apparent that the update may be seen abstractly in two different ways. Regarding the uncertain parameters

$$q : \Omega \rightarrow \mathcal{Q} \text{ as a RV on a probability space } (\Omega, \mathfrak{A}, \mathbb{P}) \quad (3)$$

where the set of elementary events is Ω , \mathfrak{A} a σ -algebra of events, and \mathbb{P} a probability measure, one set of methods performs the update by changing the probability measure \mathbb{P} and leaving the mapping $q(\omega)$ as it is, whereas the other set of methods leaves the probability measure unchanged and updates

the function $q(\omega)$. In any case, the push forward measure $q_*\mathbb{P}$ on \mathcal{Q} defined by $q_*\mathbb{P}(\mathcal{R}) := \mathbb{P}(q^{-1}(\mathcal{R}))$ for a measurable subset $\mathcal{R} \subset \mathcal{Q}$ is changed from prior to posterior. For the sake of simplicity we assume here that \mathcal{Q} —the set containing possible realisations of q —is a Hilbert space. If the parameter q is a RV, then so is the state u of the system Eq. (1). In order to avoid a profusion of notation, unless there is a possibility of confusion, we will denote the random variables q, f, u which now take values in the respective spaces $\mathcal{Q}, \mathcal{U}^*$ and \mathcal{U} with the same symbol as the previously deterministic quantities in Eq. (1).

In our overview on [29] spectral methods in identification problems we show that Bayesian identification methods [14, 36, 9, 35] are a good way to tackle the identification problem, especially when these latest developments in functional approximation methods are used. In the series of papers [25, 31, 23, 26, 29], Bayesian updating has been used in a linearised form, strongly related to the Gauss-Markov theorem [17], in ways very similar to the well-known Kalman filter [15]. This turns out to be a linearised version of *conditional expectation*. Here we want to extend this to a non-linear form, and show some examples of linear (LBU) and non-linear (NLBU) Bayesian updates.

The organisation of the remainder of the paper is as follows: in Section 2 we review the Bayesian update—classically defined via conditional probabilities—and recall the link between conditional probability measures and conditional expectation. We show how to approximate this up to any desired polynomial degree, not only the linearised version [17, 15] which was used in [25, 31, 23, 26, 29].

The numerical realisation in terms of a functional or spectral approximation—here we use the well known Wiener-Hermite chaos—is shortly sketched in Section 3. In Section 4 we then show some computational examples with the *linear version* (LBU), whereas in Section 5 we show how to compute with the non-linear version. Some concluding remarks are offered in Section 6.

2 Bayesian Updating

In the setting of Eq. (1) let us pose the following problem: the parameters $q \in \mathcal{Q}$ are uncertain or unknown. By making observations z_k at times $0 < t_1 < \dots < t_k \dots \in [0, T]$ one would like to infer what they are. But we can not observe the entity q directly—like in Plato’s cave allegory we can only see a ‘shadow’ of it, formally given by a ‘measurement operator’

$$Y : \mathcal{Q} \times \mathcal{U} \ni (q, u(t_k)) \mapsto y_k = Y(q; u(t_k)) \in \mathcal{Y}; \quad (4)$$

at least this is our model of what we are measuring. We assume that the space of possible measurements \mathcal{Y} is a vector space, which frequently may be regarded as finite dimensional, as one can only observe a finite number of quantities.

Usually the observation of the ‘truth’ \hat{y}_k will deviate from what we expect to observe even if we knew the right q as Eq. (1) is only a *model*—so there is some model error ϵ , and the measurement will be polluted by some measurement error ε . Hence we observe $z_k = \hat{y}_k + \epsilon + \varepsilon$. From this one would like to know what q and $u(t_k)$ are. For the sake of simplicity we will only consider one error term $z_k = \hat{y}_k + \varepsilon$ which subsumes all the errors.

The mapping in Eq. (4) is usually not invertible and hence the problem is called ill-posed. One way to address this is via regularisation (see e.g. [3]), but here we follow a different track. Modelling our lack-of-knowledge about q and $u(t_k)$ in a Bayesian way [36] by replacing them with a \mathcal{Q} - resp. \mathcal{U} -valued random variable (RV), the problem becomes well-posed [35]. But of course one is looking now at the problem of finding a probability distribution that best fits the data; and one also obtains a probability distribution, not just *one* pair q and $u(t_k)$. Here we focus on the use of a linear Bayesian approach [9] in the framework of ‘white noise’ analysis.

We also assume that the error $\varepsilon(\omega)$ is a \mathcal{Y} -valued RV. Please observe that although \hat{y}_k may be a deterministic quantity—the unknown ‘truth’—the model for the observed quantity $z_k(\omega) = \hat{y}_k + \varepsilon_k(\omega)$ therefore becomes a RV as well.

The mathematical setup then is as follows: we assume that Ω is a measure space with σ -algebra \mathfrak{A} and with a probability measure \mathbb{P} , and that $q : \Omega \rightarrow \mathcal{Q}$ and $u : \Omega \rightarrow \mathcal{U}$ are random variables (RVs). The corresponding *expectation* will be denoted by $\bar{q} = \mathbb{E}(q) = \int_{\Omega} q(\omega) \mathbb{P}(d\omega)$, giving the mean \bar{q} of the random variable, also denoted by $\langle q \rangle := \bar{q}$. The quantity $\tilde{q} := q - \bar{q}$ is the zero-mean or fluctuating part of the RV q . The covariance between two RVs q and u is denoted by $\text{cov}_{qu} := \mathbb{E}(\tilde{q} \otimes \tilde{u})$, the expected value of the *tensor* product of the fluctuating parts. For simplicity, we shall also require \mathcal{Q} to be a Hilbert space where each vector is a possible realisation. This is in order to allow to measure the distance between different q ’s as the norm of their difference, and to allow the operations of linear algebra to be performed.

Bayes’s theorem is commonly accepted as a consistent way to incorporate new knowledge into a probabilistic description [14, 36]. The elementary textbook statement of the theorem is about conditional probabilities

$$\mathbb{P}(I_q | M_z) = \frac{\mathbb{P}(M_z | I_q)}{\mathbb{P}(M_z)} \mathbb{P}(I_q), \quad (5)$$

where I_q is some subset of possible q ’s, and M_z is the information provided by

the measurement. This becomes problematic when the set M_z has vanishing probability measure, but if all measures involved have probability density functions (pdf), it may be formulated as ([36] Ch. 1.5)

$$\pi_q(q|z) = \frac{p(z|q)}{Z_s} p_q(q), \quad (6)$$

where p_q is the pdf of q , $p(z|q)$ is the likelihood of $z = \hat{y} + \varepsilon$ given q , as a function of q sometimes denoted by $L(q)$, and Z_s (from German *Zustandssumme*) is a normalising factor such that the conditional density $\pi_q(\cdot|z)$ integrates to unity. These terms are in direct correspondence with those in Eq. (5). Most computational approaches determine the pdfs [20, 35, 16]. Please observe that the model for the RV representing the error $\varepsilon(\omega)$ determines the likelihood functions $\mathbb{P}(M_z|I_q)$ resp. $p(z|q) = L(q)$.

However, to avoid the critical cases alluded to above, Kolmogorov already defined conditional probabilities via conditional expectation, e.g. see [2]. Given the conditional expectation $\mathbb{E}(\cdot|M_z)$, the conditional probability is easily recovered as $\mathbb{P}(I_q|M_z) = \mathbb{E}(\chi_{I_q}|M_z)$, where χ_{I_q} is the characteristic function of the subset I_q . It may be shown that this extends the simpler formulation described by Eq. (5) or Eq. (6) and is the more fundamental notion, which we examine next.

2.1 Conditional expectation

The easiest point of departure for conditional expectation in our setting is to define it not just for one piece of measurement M_z —which may not even be possible unambiguously—but for sub- σ -algebras $\mathfrak{S} \subset \mathfrak{A}$. A sub- σ -algebra \mathfrak{S} is a mathematical description of a reduced possibility of randomness, as it contains fewer events than the full algebra \mathfrak{A} . The connection with a measurement M_z is to take $\mathfrak{S} := \sigma(z)$, the σ -algebra generated by the measurement $z = Y(q) + \varepsilon$. These are all events which are consistent with possible observations of some value for z .

For RVs with finite variance—elements of $\mathcal{S} := L_2(\Omega, \mathfrak{A}, \mathbb{P})$ —the space with the sub- σ -algebra $\mathcal{S}_\infty := L_2(\Omega, \mathfrak{S}, \mathbb{P})$ is a closed subspace of the full space \mathcal{S} [2]. It represents the RVs which are possible candidates to represent the posterior, as they are consistent with any possible observation or measurement. For RVs in \mathcal{S} the conditional expectation $\mathbb{E}(\cdot|\mathfrak{S})$ is defined as the orthogonal projection onto the closed subspace \mathcal{S}_∞ , e.g. see [2]. This allows a simple geometrical interpretation: the difference between the original RV and its projection has to be perpendicular to the subspace (see Eq. (8)), and the projection minimises the distance to the original RV over the whole subspace

(see Eq. (7)). The square of this distance may be interpreted as a difference in variance, tying conditional expectation with variance minimisation; see for example [27] and the references therein for basic descriptions of conditional expectation.

As we have to deal with \mathcal{Q} -valued RVs, a bit more formalism is needed: define the space $\mathcal{Q} := \mathcal{Q} \otimes \mathcal{S}$ of \mathcal{Q} -valued RVs of finite variance, and set $\mathcal{Q}_\infty := \mathcal{Q} \otimes \mathcal{S}_\infty$ for the \mathcal{Q} -valued RVs with finite variance on the sub- σ -algebra \mathfrak{S} , representing the new information.

The Bayesian update as conditional expectation is now simply formulated:

$$\mathbb{E}(q|\mathfrak{S}) := P_{\mathcal{Q}_\infty}(q) := \arg \min_{\tilde{q} \in \mathcal{Q}_\infty} \|q - \tilde{q}\|_{\mathcal{Q}}^2, \quad (7)$$

where $P_{\mathcal{Q}_\infty}$ is the orthogonal projector onto \mathcal{Q}_∞ . The norm on the Hilbert tensor product in Eq. (7) is as usually derived from the inner product for $p = r \otimes s \in \mathcal{Q} : \langle p, p \rangle_{\mathcal{Q}} := \langle r, r \rangle_{\mathcal{Q}} \langle s, s \rangle_{\mathcal{S}}$, so that $\|p\|_{\mathcal{Q}} = \|r\|_{\mathcal{Q}} \|s\|_{\mathcal{S}}$. Already in [15] it was noted that the conditional expectation is the best estimate not only for the *loss function* ‘distance squared’, as in Eq. (7), but for a much larger class of loss functions under certain distributional constraints. However for the above loss function this is valid without any restrictions.

Requiring the derivative of the quadratic loss function in Eq. (7) to vanish—equivalently recalling the simple geometrical characterisation mentioned just before about the orthogonality—one arrives at the well-known orthogonality conditions. For later reference, we collect this result in

Proposition 1. *There is a unique minimiser to the problem in Eq. (7), denoted by $\mathbb{E}(q|\mathfrak{S}) = P_{\mathcal{Q}_\infty}(q) \in \mathcal{Q}_\infty$, and it is characterised by the orthogonality condition*

$$\forall \tilde{q} \in \mathcal{Q}_\infty : \quad \langle q - \mathbb{E}(q|\mathfrak{S}), \tilde{q} \rangle_{\mathcal{Q}} = 0. \quad (8)$$

Proof. Either by requiring the derivative of the *loss function* $\|q - \cdot\|_{\mathcal{Q}}^2$ on the closed subspace \mathcal{Q}_∞ to vanish, or by remembering that the difference between q and its best approximation from \mathcal{Q}_∞ is orthogonal to that subspace [17], one arrives immediately at Eq. (8). The existence and uniqueness of the best approximation follows from the fact that $\mathcal{Q}_\infty = \mathcal{Q} \otimes \mathcal{S}_\infty$ is a closed subspace (as \mathcal{S}_∞ is a closed subspace), hence a closed convex set, and the loss function is continuous and strictly convex. Equivalently, this says that the projection $P_{\mathcal{Q}_\infty}$ is continuous and orthogonal, i.e. its norm is equal to unity.

Alternatively, we may invoke the *Lax-Milgram* lemma for Eq. (8), coerciveness and continuity are trivially satisfied on the subspace \mathcal{Q}_∞ , which is closed and hence a *Hilbert* space. \square

Let us remark that *Pythagoras's* theorem implies that

$$\|P_{\mathcal{Q}_\infty}(q)\|_{\mathcal{Q}}^2 = \|q\|_{\mathcal{Q}}^2 - \|q - P_{\mathcal{Q}_\infty}(q)\|_{\mathcal{Q}}^2.$$

To continue, note that the *Doob-Dynkin* lemma [2] assures us that if a RV like $\mathbb{E}(q|\mathfrak{S})$ is in the subspace \mathcal{Q}_∞ , then $\mathbb{E}(q|\mathfrak{S}) = \varphi(z)$ for some $\varphi \in L_0(\mathcal{Y}; \mathcal{Q})$, the space of measurable functions from $\mathcal{Y} := \mathcal{Y} \otimes \mathcal{S}$ to \mathcal{Q} . We state this key fact and the resulting new characterisation of the conditional expectation in

Proposition 2. *The subspace $\mathcal{Q}_\infty = \mathcal{Q} \otimes \mathcal{S}_\infty$ is given by*

$$\mathcal{Q}_\infty = \overline{\text{span}}\{\varphi \mid \varphi(\phi, q) := \phi(Y(q) + \varepsilon); \phi \in L_0(\mathcal{Y}; \mathcal{Q}) \text{ s.t. } \varphi \in \mathcal{Q}\}. \quad (9)$$

Finding the conditional expectation may be seen as rephrasing Eq. (7) as:

$$\mathbb{E}(q|\sigma(Y)) := P_{\mathcal{Q}_\infty}(q) = \arg \min_{\phi \in L_0(\mathcal{Y}; \mathcal{Q})} \|q - \varphi(\phi, q)\|_{\mathcal{Q}}^2. \quad (10)$$

Proof. Follows directly from the Doob-Dynkin lemma. \square

Then $q_a := P_{\mathcal{Q}_\infty}(q)$ is called the *updated, analysis, assimilated, or posterior* value, incorporating the new information. This is the Bayesian update expressed in terms of RVs instead of measures. It is the estimate of the unknown parameters q after the measurement has been performed.

2.2 Approximation of the conditional expectation

Computationally we will not be able to deal with the *whole* space \mathcal{Q}_∞ , so we look at the effect of approximations. Assume that $L_0(\mathcal{Y}; \mathcal{Q})$ in Eq. (10) is approximated by subspaces $L_{0,n} \subset L_0(\mathcal{Y}; \mathcal{Q})$, where $n \in \mathbb{N}$ is a parameter describing the level of approximation and $L_{0,n} \subset L_{0,m}$ if $n < m$, such that the subspaces

$$\mathcal{Q}_n = \text{span}\{\varphi(\phi, q) \mid \phi \in L_{0,n} \subset L_0(\mathcal{Y}; \mathcal{Q}) \text{ s.t. } \varphi \in \mathcal{Q}\} \subset \mathcal{Q}_\infty \quad (11)$$

are closed and their union is dense $\overline{\bigcup_n \mathcal{Q}_n} = \mathcal{Q}_\infty$, a consistency condition. From *C  a's* lemma we immediately get:

Proposition 3. *Define*

$$P_{\mathcal{Q}_n}(q) := \arg \min_{\phi \in L_{0,n}} \|q - \varphi(\phi, q)\|_{\mathcal{Q}}^2. \quad (12)$$

Then the sequence $q_{a,n} := P_{\mathcal{Q}_n}(q)$ converges to $q_a := P_{\mathcal{Q}_\infty}(q)$:

$$\lim_{n \rightarrow \infty} \|q_a - q_{a,n}\|_{\mathcal{Q}}^2 = 0. \quad (13)$$

Proof. Well-posedness is a direct consequence of Proposition 1, and the $P_{\mathcal{Q}_n}$ are orthogonal projections onto the subspaces \mathcal{Q}_n , hence their norms are all equal to unity—a stability condition. Application of C  a’s lemma then directly yields Eq. (13). \square

Here we choose the subspaces of polynomials up to degree n for the purpose of approximation, i.e.

$$\mathcal{Q}_n := \text{span}\{\varphi \in \mathcal{Q} \mid \varphi(\psi_n, q), \psi_n \text{ a } n^{\text{th}} \text{ degree polynomial}\},$$

and we remark that in case \mathcal{Y} is finite-dimensional—the usual case—then the space of n^{th} degree polynomials is a closed space. We may write this as

$$\psi_n(z) := {}^0H + {}^1Hz + \cdots + {}^kH z^{\vee k} + \cdots + {}^nH z^{\vee n}, \quad (14)$$

where ${}^kH \in \mathcal{L}_s^k(\mathcal{Y}, \mathcal{Q})$ is symmetric and k -linear; and $z^{\vee k} := \overbrace{z \vee \cdots \vee z}^k := \text{Sym}(z^{\otimes k})$ is the symmetric tensor product of the z ’s taken k times with itself. Let us remark here that the form of Eq. (14), given in monomials, is numerically not a good form—except for very low n —and straightforward use in computations is not recommended. The relation Eq. (14) could be re-written in some orthogonal polynomials—or in fact any other system of multi-variate functions; this generalisation will be published elsewhere. For the sake of conceptual simplicity, we stay with Eq. (14) and then have that

$$q_{a,n}({}^0H, \dots, {}^nH) := \psi_n(z) := {}^0H + \cdots + \cdots + {}^nH z^{\vee n} \quad (15)$$

is a function of the maps kH . The stationarity or orthogonality condition Eq. (8) can then be written in terms of the kH . We need the following abbreviations for any $k, \ell \in \mathbb{N}_0$:

$$\langle p \otimes v^{\vee k} \rangle := \mathbb{E} (p \otimes v^{\vee k}) = \int_{\Omega} p(\omega) \otimes v(\omega)^{\vee k} \mathbb{P}(\text{d}\omega)$$

and

$${}^kH \langle z^{\vee(\ell+k)} \rangle := \langle z^{\vee \ell} \vee ({}^kH z^{\vee k}) \rangle = \mathbb{E} \left(z^{\vee \ell} \vee ({}^kH z^{\vee k}) \right).$$

We may then characterise the kH in the following way:

Theorem 4. *With $q_{a,n}$ given by Eq. (15), the stationarity condition Eq. (8) becomes for any $n \in \mathbb{N}_0$ ($\delta_{(\ell H)}$ the G  teaux derivative w.r.t. ${}^{\ell}H$):*

$$\forall \ell = 0, \dots, n : \quad \delta_{(\ell H)} \|q - q_a({}^0H, \dots, {}^nH)\|_{\mathcal{Q}}^2 = 0, \quad (16)$$

The case $n = 1$ in Eq. (17) or Eq. (18) is more interesting, allowing up to *linear* terms:

$$\begin{aligned} {}^0H + {}^1H \langle z \rangle &= \langle q \rangle \\ {}^0H \langle z \rangle + {}^1H \langle z \otimes z \rangle &= \langle q \otimes z \rangle. \end{aligned}$$

Remembering that $[\text{cov}_{qz}] = \langle q \otimes z \rangle - \langle q \rangle \otimes \langle z \rangle$ and analogous for $[\text{cov}_{zz}]$, one obtains by tensor multiplication in Eq. (19) with $\langle z \rangle$ and symbolic Gaussian elimination the Eq. (20).

$${}^0H = \langle q \rangle - {}^1H \langle z \rangle \quad (19)$$

$${}^1H (\langle z \otimes z \rangle - \langle z \rangle \otimes \langle z \rangle) = {}^1H [\text{cov}_{zz}] = \langle q \otimes z \rangle - \langle q \rangle \otimes \langle z \rangle = [\text{cov}_{qz}]. \quad (20)$$

This gives

$${}^1H = [\text{cov}_{qz}] [\text{cov}_{zz}]^{-1} =: K \quad (21)$$

$${}^0H = \langle q \rangle - [\text{cov}_{qz}] [\text{cov}_{zz}]^{-1} \langle z \rangle. \quad (22)$$

where K in Eq. (21) is the well-known *Kalman* gain operator [15], so that finally

$$q_a = {}^0H + {}^1H z = \langle q \rangle + [\text{cov}_{qz}] [\text{cov}_{zz}]^{-1} (z - \langle z \rangle) = \langle q \rangle + K (z - \langle z \rangle). \quad (23)$$

This is called the *linear* Bayesian update (LBU). It is important to see Eq. (23) as a symbolic expression, especially the inverse $[\text{cov}_{zz}]^{-1}$ indicated there should not really be computed, especially when $[\text{cov}_{zz}]$ is ill-conditioned or close to singular. The inverse can in that case be replaced by the *pseudo-inverse*, or rather the computation of K , which is in linear algebra terms a *least-squares* approximation, should be done with orthogonal transformations and not by elimination. We will not dwell on these well-known matters here.

The case $n = 2$ can still be solved symbolically, the system to be solved is from Eq. (17) or Eq. (18):

$$\begin{aligned} {}^0H + {}^1H \langle z \rangle + {}^2H \langle z^{\otimes 2} \rangle &= \langle q \rangle \\ {}^0H \langle z \rangle + {}^1H \langle z^{\otimes 2} \rangle + {}^2H \langle z^{\otimes 3} \rangle &= \langle q \otimes z \rangle \\ {}^0H \langle z^{\otimes 2} \rangle + {}^1H \langle z^{\otimes 3} \rangle + {}^2H \langle z^{\otimes 4} \rangle &= \langle q \otimes z^{\otimes 2} \rangle. \end{aligned}$$

After some symbolic elimination steps one obtains

$$\begin{aligned} {}^0H + {}^1H \langle z \rangle + {}^2H \langle z^{\otimes 2} \rangle &= \langle q \rangle \\ 0 + {}^1H + {}^2H \mathbf{F} &= K \\ 0 + 0 + {}^2H \mathbf{G} &= \mathbf{E}, \end{aligned}$$

with the Kalman gain operator $K \in (\mathcal{Q} \otimes \mathcal{Y})^*$ from Eq. (21), the third order tensors $\mathbf{F} \in (\mathcal{Y}^{\otimes 3})^*$ given in Eq. (24), and $\mathbf{E} \in (\mathcal{Q} \otimes \mathcal{Y}^{\otimes 2})^*$ given in Eq. (25), and the fourth order tensor $\mathbf{G} \in (\mathcal{Y}^{\otimes 4})^*$ given in Eq. (26):

$$\mathbf{F} = (\langle z^{\otimes 3} \rangle - \langle z^{\otimes 2} \rangle \otimes \langle z \rangle) \cdot [\text{cov}_{zz}]^{-1}, \quad (24)$$

$$\mathbf{E} = \langle q \otimes z^{\otimes 2} \rangle - \langle q \rangle \otimes \langle z^{\otimes 2} \rangle - K \cdot (\langle z^{\otimes 3} \rangle - \langle z \rangle \otimes \langle z^{\otimes 2} \rangle) \quad (25)$$

$$\mathbf{G} = (\langle z^{\otimes 4} \rangle - \langle z^{\otimes 2} \rangle^{\otimes 2}) - \mathbf{F} \cdot (\langle z^{\otimes 3} \rangle - \langle z \rangle \otimes \langle z^{\otimes 2} \rangle), \quad (26)$$

where the single central dot ‘ \cdot ’ denotes as usual a contraction over the appropriate indices, and a colon ‘ $:$ ’ a double contraction. From this one easily obtains the solution

$${}^2H = \mathbf{E} : \mathbf{G}^{-1} \quad (27)$$

$${}^1H = K - \mathbf{E} : \mathbf{G}^{-1} : \mathbf{F} \quad (28)$$

$${}^0H = \langle q \rangle - (K - \mathbf{E} : \mathbf{G}^{-1} : \mathbf{F}) \cdot \langle z \rangle - \mathbf{E} : \mathbf{G}^{-1} : \langle z^{\otimes 2} \rangle. \quad (29)$$

2.3 Prior information and mappings

In case one has *prior* information \mathcal{Q}_f and a prior estimate $q_f(\omega)$ (forecast), and a new measurement z comes in generating via $\sigma(z)$ a subspace $\mathcal{Q}_y \subset \mathcal{Q}$, one now needs a projection onto $\mathcal{Q}_a = \mathcal{Q}_f + \mathcal{Q}_y$, with reformulation as an orthogonal direct sum

$$\mathcal{Q}_a = \mathcal{Q}_f + \mathcal{Q}_y = \mathcal{Q}_f \oplus (\mathcal{Q}_y \cap \mathcal{Q}_f^\perp) = \mathcal{Q}_f \oplus \mathcal{Q}_\infty,$$

in order not to update twice with the nonzero part of $\mathcal{Q}_y \cap \mathcal{Q}_f$.

The *update / conditional expectation / assimilated* value is

$$q_a = q_f + P_{\mathcal{Q}_\infty} q = q_f + q_\infty,$$

where q_∞ is the *innovation*, the orthogonal projection onto \mathcal{Q}_∞ . This is reminiscent of Eq. (23), where the term $\langle q \rangle$ may be regarded as the *prior* information (before any measurement is performed) and replaced here by q_f , and the innovation there is $K(z - \langle z \rangle)$, which is here represented by q_∞ .

The $n = 1$ version of Theorem 4 is well-known, and in conjunction with what was just stated about prior information is of considerable practical importance; it is an extension of the *Kalman filter* [15, 17, 27]. We rephrase this generalisation of the well-known *Gauss-Markov* theorem from [17] Chapter 4.6, Theorem 3:

Theorem 5. *The update $q_{a,1}$, minimising $\|q - \cdot\|_{\mathcal{Q}}^2$ over all elements generated by affine mappings (the up to $n = 1$ case of Theorem 4) of the measurement in the case with prior information q_f and predicted measurement $z = Y(q_f) + \varepsilon$ is given from the observation \hat{z} by*

$$q_{a,1} = q_f + K(\hat{z} - z), \quad (30)$$

where the notation $q_{a,1}$ is according to Eq. (15), and the operator K is the Kalman gain from Eq. (23).

This update is in some ways very similar to the ‘Bayes linear’ approach [9]. We point out that q_a and q_f are RVs, i.e. this is an equation in $\mathcal{Q} = \mathcal{Q} \otimes \mathcal{S}$, whereas the traditional Kalman filter—which looks superficially just like Eq. (30) is an equation in \mathcal{Q} . Observe that $z = Y(q_f) + \varepsilon$ and that the error term is a RV. Hence the quantity z is an RV, and Eq. (30) is an equation between RVs. If the mean is taken in Eq. (30), one obtains the familiar Kalman filter formula [15] for the update of the mean, and one may show [25] that Eq. (30) also contains the Kalman update for the covariance, i.e. the Kalman filter is a low-order part of Eq. (30). The computational strategy is now to replace and approximate the—only abstractly given—computation of q_a by the practically possible calculation of $q_{a,n}$ as in Eq. (15). This means that we approximate q_a by $q_{a,n}$ by using $\mathcal{Q}_n \subset \mathcal{Q}_\infty$, and rely on Proposition 3. This corresponds to some loss of information from the measurement, but yields a manageable computation. If the assumptions of Proposition 3 are satisfied, then one can expect for n large enough that the terms in Eq. (15) converge to zero, thus providing an error indicator on when a sufficient accuracy has been reached.

In case the space generated by the measurements is not dense in \mathcal{Q} a residual error will thus remain, as the measurements do not contain enough information to resolve our lack of knowledge about q . Anyway, finding q is limited by the presence of the error ε , as obviously the error influences the update in Eq. (30). If the measurement operator is approximated in some way—as it will be in the computational examples to follow—this will introduce a new error, further limiting the resolution.

It is maybe worthwhile to pursue the following idea: The mapping we try to approximate $q \mapsto P_{\mathcal{Q}_\infty}(q)$ is an orthogonal projection, hence linear. This carries with it several suggestions on how to change the update process.

Given a couple q and measurement operator $y = Y(q)$, one may change the arrangement by mappings of q or y . On one hand one may consider a—preferably—injective map $\Theta : \mathcal{T} \rightarrow \mathcal{Q}$ and choose $p = \Theta^{-1}(q) \in \mathcal{T}$ as parameter, the measurement operator is then $\tilde{Y}(p) = Y(\Theta(p))$. This may be useful as we want to perform essentially linear operations on q like the above

mentioned projection and linear approximations to it, and if the set where q ‘lives’ is not a linear set, this is problematic. We will come across this example in Section 4, where q is positive—or a symmetric positive definite tensor—and hence ‘lives’ on an *open* cone in a vector space. There we will choose $\Theta = \exp$, and in [29] we give some arguments why this may be meaningful, as this transformation puts us in the tangent space of the positive cone, which is a *linear* space.

On the other hand looking again at a given pair q and $Y(q)$, the linear map $q \mapsto P_{\mathcal{Q}\infty}(q)$ is approximated by $\psi_n(y) = \psi_n(Y(q))$ from Eq. (14)—neglecting measurement error for the moment. This means that when Y is nonlinear in q , the update map ψ_n from Eq. (14) has to somehow ‘straighten’ the nonlinearity out. This opens the possibility to make the update ‘easier’: we update not from $Y(q)$, but from $\Xi(Y(q))$, where $\Xi : \mathcal{Q} \rightarrow \mathcal{X}$ is chosen so that the composition $\Xi \circ Y$ is ‘less nonlinear’. This means that in the computation of ψ_n , we try to minimise the error of $\psi_n \circ \Xi$. Finding a suitable Ξ —in some way an ‘inverse’ of Y —is not easy. Anyway, some preliminary examples where Ξ has been chosen heuristically were very promising and will be reported elsewhere.

If the mapping Y is not injective, then of course this can not be ‘ironed out’ by any mapping Ξ , as we would need to undo the loss of information from Y being not injective—another sign of ill-posedness. The mapping Ξ could be speculatively made into a set-valued mapping to achieve this, but we would have, for a certain y , to find all $q \in Y^{-1}(y)$ to construct Ξ such that it distinguishes them, not an easy task.

We close this section by pointing out a little example connected to these considerations—suggested to us by [34]—which is a bit disturbing and shows the possible problems involved and that one has to be a bit careful: Assume that $q_f = \theta$ is a single centred Gaussian variable with variance ζ^2 , and that the measurement operator is $Y(q) = q^2$, i.e. all information about the sign is lost. Assume that $\varepsilon = z - Y(q)$ is independent of q and also centred. Taking first the linear Bayesian update (LBU) from Theorem 5 defined in Eq. (21), we have that—as $\mathbb{E}(q) = 0$ and $\mathbb{E}(q^2) = \zeta^2$

$$[\text{cov}_{q,z}] = [\text{cov}_{q,y}] = \mathbb{E}((\theta - 0)(\theta^2 - \zeta^2)) = \mathbb{E}(\theta^3 - \theta\sigma^2) = 0,$$

and hence $K = [\text{cov}_{q,z}][\text{cov}_{z,z}]^{-1} = 0$, and the LBU Eq. (30) will *not* change anything; $q_{a,1} = q_f$. Looking for the reason for this, we observe that in the system Eq. (17) in Theorem 4—or in Eq. (18)—the right-hand-side (rhs) is

$\langle q \otimes z^{\vee k} \rangle$ in the k -th equation. In our case this evaluates to

$$\begin{aligned} \langle q \otimes z^{\vee k} \rangle &= \mathbb{E}(q \otimes z^{\vee k}) = \mathbb{E}(q(q^2 + \varepsilon)^k) = \\ &= \mathbb{E}\left(q \left(\sum_{i=0}^k c_i q^{2i} \varepsilon^{k-i} \right)\right) = \sum_{i=0}^k c_i \mathbb{E}(\theta^{2i+1}) \mathbb{E}(\varepsilon^{k-i}) = 0, \end{aligned}$$

as $\mathbb{E}(\theta^{2i+1}) = 0$ for any $i \in \mathbb{N}_0$. Obviously the c_i are the binomial coefficients. This means that in Eq. (17) or Eq. (18) the rhs vanishes *identically* for any $n \in \mathbb{N}$, and hence all ${}^k H$ will vanish too; i.e. no matter what polynomial update we take, always $\psi_n \equiv 0$, and hence $q_{a,n} = q_f$ for all $n \in \mathbb{N}$. The loss of information about the sign is so intertwined with the measurement that no update of the form Eq. (14) can undo it!

If we now come back to the first idea of choosing a map Θ as sketched above, we might chose $p = |q|$, then $\hat{Y}(p) = p^2 = |q|^2 = Y(q)$; which means we do not care about the sign, as information about the sign is lost anyway. The rhs now is—again neglecting measurement error for the sake of simplicity

$$\mathbb{E}(p \otimes z^{\vee k}) = \mathbb{E}(p^{2k+1}) = \mathbb{E}(|q|^{2k+1}) = \mathbb{E}(|\theta|^{2k+1}) = \zeta^{2k+1} 2^k k! \sqrt{\frac{2}{\pi}},$$

as these are simply the moments of the *half-normal* or χ -distribution, and hence one could now compute a polynomial update map ψ_n for any n .

One might think that in the formula for the Bayesian update of densities Eq. (6) this kind of problem does not appear, but the difficulty comes when one has to compute the *likelihood* $p(z|q)$ in Eq. (6). Given a measurement $z = y + \varepsilon$ we have to find *all* q which might have produced it, and this means that one has to compute the set $Y^{-1}(y)$; so this is where the difficulty appears then!

We now turn to some examples where we identify parameters in models of varying complexity. In Section 4 we will show several examples for the case of $n = 1$ for the update map ψ_n , and in Section 5 an example for the case $n = 2$.

3 Numerical realisation

In the instances where we want to employ the theory detailed in the previous Section 2, the spaces \mathcal{U} and \mathcal{Q} are usually infinite dimensional, as is the space $\mathcal{S} = L_2(\Omega)$. For an actual computation they have to be discretised or approximated by finite dimensional spaces. In our examples we will chose finite element discretisations and corresponding subspaces. Hence

let $\mathcal{Q}_M := \text{span} \{ \varrho_m : m = 1, \dots, M \} \subset \mathcal{Q}$ be an M -dimensional subspace with basis $\{ \varrho_m \}_{m=1}^M$. An element of \mathcal{Q}_M will be represented by the vector $\mathbf{q} = [q^1, \dots, q^M]^T \in \mathbb{R}^M$ such that $\sum_{m=1}^M q^m \varrho_m \in \mathcal{Q}_M$. To avoid a profusion of notations, the corresponding random vector in $\mathbb{R}^M \otimes \mathcal{S}$ will also be denoted by \mathbf{q} . The norm $\|\mathbf{q}\|_M$ to take on \mathbb{R}^M results from the inner product $\langle \mathbf{q}_1 | \mathbf{q}_2 \rangle_M := \mathbf{q}_1^T \mathbf{Q} \mathbf{q}_2$ with $\mathbf{Q} = (\langle \varrho_m | \varrho_n \rangle_{\mathcal{Q}})$, the Gram matrix of the basis. We will later choose an orthonormal basis, so that $\mathbf{Q} = \mathbf{I}$ is the identity matrix. Similarly, on $\mathcal{Q}_M = \mathbb{R}^M \otimes \mathcal{S}$ the inner product is $\langle \mathbf{q}_1 | \mathbf{q}_2 \rangle_{\mathcal{Q}_M} := \mathbb{E}(\langle \mathbf{q}_1 | \mathbf{q}_2 \rangle_M)$. The space of possible measurements can usually be taken to be finite dimensional (here $= R$), whose elements are similarly represented by a vector of coefficients $\mathbf{z} \in \mathbb{R}^R$.

On \mathbb{R}^M , representing \mathcal{Q}_M , the Kalman gain operator in Theorem 5 in Eq. (30) becomes a matrix $\mathbf{K} \in \mathbb{R}^{M \times R}$. Then the update corresponding to Eq. (30) is

$$\mathbf{q}_a = \mathbf{q}_f + \mathbf{K}(\hat{\mathbf{z}} - \mathbf{z}), \text{ with } \mathbf{K} = \mathbf{C}_{q,z} \mathbf{C}_{z,z}^{-1}. \quad (31)$$

Here the covariances are $\mathbf{C}_{q,z} := \mathbb{E}(\tilde{\mathbf{q}} \tilde{\mathbf{z}}^T) = \mathbb{E}(\tilde{\mathbf{q}} \otimes \tilde{\mathbf{z}})$, and similarly for $\mathbf{C}_{z,z}$. Often the measurement error ε is independent of \mathbf{q} — actually uncorrelated would be *sufficient*—hence $\mathbf{C}_{z,z} = \mathbf{C}_{y,y} + \mathbf{C}_{\varepsilon,\varepsilon}$ and $\mathbf{C}_{q,z} = \mathbf{C}_{q,y}$. We once more recall our comments in Subsection 2.2 following Eq. (23) regarding the inverse which also appears in Eq. (31). Recall that usually the error model involves a regular covariance $\mathbf{C}_{\varepsilon,\varepsilon}$, so that $\mathbf{C}_{z,z} = \mathbf{C}_{y,y} + \mathbf{C}_{\varepsilon,\varepsilon}$ is at least theoretically regular.

It is important to emphasise that the theory presented in the forgoing Section 2 is independent of any discretisation. But one usually can still not numerically compute with objects like $\mathbf{q} \in \mathcal{Q}_M = \mathbb{R}^M \otimes \mathcal{S}$, as $\mathcal{Q} = L_2(\Omega)$ is normally an infinite dimensional space and has to be discretised. One well-known possibility are samples, i.e. the RV $\mathbf{q}(\omega)$ is represented by its value at certain points ω_z , and the points usually come from some quadrature rule. The well-known Monte Carlo (MC) method uses random samples, the quasi-Monte Carlo (QMC) method uses low discrepancy samples, and other rules like sparse grids (Smolyak rule) are possible. Using MC samples in the context of the linear update Eq. (30) is known as the *Ensemble Kalman Filter* (EnKF), see [29] for a general overview in this context, and [4, 5] for a thorough description and analysis. This method is conceptually fairly simple and is currently a favourite for problems where the computation of the predicted measurement $\mathbf{y}_f(\omega_z)$ is difficult or expensive. It needs far fewer samples for meaningful results than MCMC, but on the other hand it uses the linear approximation inherent in Eq. (31).

Here we want to use so-called *functional* or *spectral* approximations, so similarly as for \mathcal{Q}_M , we pick a finite set of linearly independent vectors in

\mathcal{S} . As $\mathcal{S} = L_2(\Omega)$, these abstract vectors are in fact RVs with finite variance. Here we will use the best known example, namely *Wiener's polynomial chaos* expansion (PCE) as basis [37, 8, 12, 13, 19, 21], this allows us to use Eq. (31) without sampling, see [29, 25, 31, 23, 26], and also [33, 1].

The PCE is an expansion in multivariate *Hermite polynomials* [8, 12, 13, 19, 21]; we denote by $H_{\alpha}(\theta) = \prod_{k \in \mathbb{N}} h_{\alpha_k}(\theta_k) \in \mathcal{S}$ the multivariate polynomial in standard independent Gaussian RVs $\theta(\omega) = (\theta_1(\omega), \dots, \theta_k(\omega), \dots)_{k \in \mathbb{N}}$, where h_j is the usual univariate Hermite polynomial, and $\alpha = (\alpha_1, \dots, \alpha_k, \dots)_{k \in \mathbb{N}} \in \mathcal{N} := \mathbb{N}_0^{(\mathbb{N})}$ is a multi-index of generally infinite length but with only finitely many entries non-zero. As $h_0 \equiv 1$, the infinite product is effectively finite and always well-defined.

The *Cameron-Martin* theorem assures us [12, 19, 13] that the set of these polynomials is dense in $\mathcal{S} = L_2(\Omega)$, and in fact $\{H_{\alpha}/\sqrt{(\alpha)!}\}_{\alpha \in \mathcal{N}}$ is a complete orthonormal system (CONS), where $\alpha! := \prod_{k \in \mathbb{N}} (\alpha_k!)$ is the product of the individual factorials, also well-defined as except for finitely many k one has $\alpha_k! = 0! = 1$. So we may write $\mathbf{q}(\omega) = \sum_{\alpha \in \mathcal{N}} \mathbf{q}^{\alpha} H_{\alpha}(\theta(\omega))$ with $\mathbf{q}^{\alpha} \in \mathbb{R}^M$, and similarly for \mathbf{z} and all other RVs. In this way the RVs are expressed as functions of other, known RVs θ —hence the name *functional* approximation—and not through samples.

The space \mathcal{S} may now be discretised by taking a finite subset $\mathcal{J} \subset \mathcal{N}$ of size $J = |\mathcal{J}|$, and setting $\mathcal{S}_J = \text{span} \{H_{\alpha} : \alpha \in \mathcal{J}\} \subset \mathcal{S}$. The orthogonal projection P_J onto \mathcal{S}_J is then simply

$$P_J : \mathcal{Q}_M \otimes \mathcal{S} \ni \sum_{\alpha \in \mathcal{N}} \mathbf{q}^{\alpha} H_{\alpha} \mapsto \sum_{\alpha \in \mathcal{J}} \mathbf{q}^{\alpha} H_{\alpha} \in \mathcal{Q}_M \otimes \mathcal{S}_J. \quad (32)$$

We then take Eq. (31) and rewrite it as

$$\mathbf{q}_a = \mathbf{q}_f + \mathbf{K}(\mathbf{z} - \mathbf{y}_f) = \quad (33)$$

$$\sum_{\alpha \in \mathcal{N}} \mathbf{q}_a^{\alpha} H_{\alpha}(\theta) = \sum_{\alpha \in \mathcal{N}} (\mathbf{q}_f^{\alpha} + \mathbf{K}(\mathbf{z}^{\alpha} - \mathbf{y}_f^{\alpha})) H_{\alpha}(\theta). \quad (34)$$

Projecting both sides of Eq. (34) is very simple and results in

$$\sum_{\alpha \in \mathcal{J}} \mathbf{q}_a^{\alpha} H_{\alpha} = \sum_{\alpha \in \mathcal{J}} (\mathbf{q}_f^{\alpha} + \mathbf{K}(\mathbf{z}^{\alpha} - \mathbf{y}_f^{\alpha})) H_{\alpha}. \quad (35)$$

Obviously the projection P_J commutes with the Kalman operator \mathbf{K} and hence with its finite dimensional analogue \mathbf{K} . One may actually concisely write Eq. (35) as

$$P_J \mathbf{q}_a = P_J \mathbf{q}_f + P_J \mathbf{K}(\mathbf{z} - \mathbf{y}_f) = P_J \mathbf{q}_f + \mathbf{K}(P_J \mathbf{z} - P_J \mathbf{y}_f). \quad (36)$$

Elements of the discretised space $\mathcal{Q}_{M,J} = \mathcal{Q}_M \otimes \mathcal{S}_J \subset \mathcal{Q}$ thus may be written as $\sum_{m=1}^M \sum_{\alpha \in \mathcal{J}} q^{\alpha,m} \varrho_m H_\alpha$. The tensor representation is $\mathbf{q} := (q^{\alpha,m}) = \sum_{\alpha \in \mathcal{J}} \mathbf{q}^\alpha \otimes \mathbf{e}^\alpha$, where the \mathbf{e}^α are the unit vectors in \mathbb{R}^J , may be used to express Eq. (35) or Eq. (36) succinctly as

$$\mathbf{q}_a = \mathbf{q}_f + \mathbf{K}(\mathbf{z} - \mathbf{y}_f), \quad (37)$$

again an equation between the tensor representations of some RVs, where $\mathbf{K} = \mathbf{K} \otimes \mathbf{I}$ with \mathbf{K} from Eq. (31). Hence the update equation is naturally in a tensorised form. This is how the update can finally be computed in the PCE representation without any sampling [29, 25, 30, 23]. Analogous statements hold for the forms of the update Eq. (14) with higher order terms $n > 1$, and do not have to be repeated here. Let us remark that these updates go very seamlessly with very efficient methods for sparse or low-rank approximation of tensors, c.f. the monograph [10] and the literature therein. These methods are PCE-forms of the Bayesian update, and in particular the Eq. (37), because of its formal affinity to the Kalman filter (KF), may be called the polynomial chaos expansion based Kalman filter (PCEKF).

It remains to say how to compute the terms ${}^k H$ in the update equation Eq. (14)—or rather the terms in the defining Eq. (17) in Theorem 4—in this approach. Given the PCEs of the RVs, this is actually quite simple as any moment can be computed directly from the PCE [21, 25, 31]. A typical term $\langle z^{\vee k} \rangle = \langle \text{Sym}(z^{\otimes k}) \rangle = \text{Sym}(\langle z^{\otimes k} \rangle)$ in the operator matrix Eq. (17), where $\mathbf{z} = \sum_{\alpha} \mathbf{z}^\alpha H_\alpha(\boldsymbol{\theta})$, may be computed through

$$\begin{aligned} \langle z^{\otimes k} \rangle &= \mathbb{E} \left(\bigotimes_{i=1}^k \sum_{\alpha_i} (z^{\alpha_i} H_{\alpha_i}) \right) = \\ &= \mathbb{E} \left(\sum_{\alpha_1, \dots, \alpha_k} \bigotimes_{i=1}^k z^{\alpha_i} \prod_{i=1}^k H_{\alpha_i} \right) = \sum_{\alpha_1, \dots, \alpha_k} \bigotimes_{i=1}^k z^{\alpha_i} \mathbb{E} \left(\prod_{i=1}^k H_{\alpha_i} \right) \end{aligned} \quad (38)$$

As here the H_α are *polynomials*, the last expectation in Eq. (38) is finally over products of powers of pairwise independent normalised Gaussian variables, which actually may be done analytically [12, 19, 13]. But some simplifications come from remembering that $\mathbf{z}^0 = \mathbb{E}(\mathbf{z}) = \bar{\mathbf{z}}$, $H_0 \equiv 1$, the orthogonality relation $\langle H_\alpha | H_\beta \rangle = \delta_{\alpha,\beta} \alpha!$, and that the Hermite polynomials are an *algebra*. Hence $H_\alpha H_\beta = \sum_{\gamma} c_{\alpha,\beta}^\gamma H_\gamma$, where the *structure coefficients* $c_{\alpha,\beta}^\gamma$ are known analytically [19, 21, 25, 31].

Similarly, for a typical right-hand-side term $\langle q \otimes z^{\vee k} \rangle = \langle q \otimes \text{Sym}(z^{\otimes k}) \rangle$

in Eq. (17) with $\mathbf{q} = \sum_{\beta} \mathbf{q}^{\beta} H_{\beta}(\boldsymbol{\theta})$ one has

$$\langle q \otimes \text{Sym}(z^{\otimes k}) \rangle = \sum_{\beta, \alpha_1, \dots, \alpha_k} \mathbf{q} \otimes \text{Sym} \left(\bigotimes_{i=1}^k z^{\alpha_i} \right) \mathbb{E} \left(H_{\beta} \prod_{i=1}^k H_{\alpha_i} \right). \quad (39)$$

As these relations may seem a bit involved—they are actually just a bit intricate combination of *known* terms—we show here how simple they become for the case of the covariance needed in the linear update formula Eq. (30) or rather Eq. (31):

$$C_{z,z} = \sum_{\alpha \in \mathcal{N}, \alpha \neq 0} (\alpha!) \mathbf{q}^{\alpha} \otimes \mathbf{z}^{\alpha} \approx \sum_{\alpha \in \mathcal{J}, \alpha \neq 0} (\alpha!) \mathbf{z}^{\alpha} \otimes \mathbf{z}^{\alpha}, \quad (40)$$

$$C_{q,z} = \sum_{\alpha \in \mathcal{N}, \alpha \neq 0} (\alpha!) \mathbf{q}^{\alpha} \otimes \mathbf{z}^{\alpha} \approx \sum_{\alpha \in \mathcal{J}, \alpha \neq 0} (\alpha!) \mathbf{q}^{\alpha} \otimes \mathbf{z}^{\alpha}. \quad (41)$$

Looking for example at Eq. (31) and our setup as explained in Section 1, we see that the coefficients of $\mathbf{z} = \sum_{\alpha} \mathbf{z}^{\alpha} H_{\alpha}$ or rather those of $\mathbf{y} = \sum_{\alpha} \mathbf{y}^{\alpha} H_{\alpha} = \mathbf{Y}(\mathbf{q})$ have to be computed from those of $\mathbf{q} = \sum_{\beta} \mathbf{q}^{\beta} H_{\beta}$. This propagation of uncertainty through the system is known as *uncertainty quantification* (UQ), e.g. [21] and the references therein. For the sake of brevity, we will not touch further on this subject, which nevertheless is the bedrock on which we built the whole computational procedure.

We next concentrate in Section 4 on examples of updating with ψ_n for the case $n = 1$ in Eq. (14), whereas in Section 5 an example for the case $n = 2$ in Eq. (14) will be shown.

4 The linear Bayesian update

All the examples in this section have been computed with the case $n = 1$ of up to linear terms in Eq. (14), i.e. this is the LBU with PCEKF. As the traditional Kalman filter is highly geared towards Gaussian distributions [15], and also its Monte Carlo variant EnKF which was mentioned in Section 3 tilts towards Gaussianity, we start with a case—already described in [25]—where the the quantity to be identified has a strongly non-Gaussian distribution, shown in black—the ‘truth’—in Fig. 1. The operator describing the system is the identity—we compute the quantity directly, but there is a Gaussian measurement error. The ‘truth’ was represented as a 12th degree PCE. We use the methods as described in Section 3, and here in particular the Eq. (31) and Eq. (37), the PCEKF.

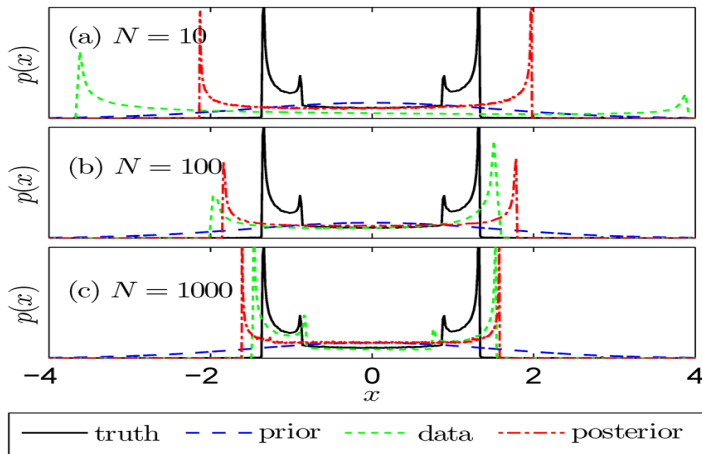


Figure 1: pdfs for linear Bayesian update

The update is repeated several times (here ten times) with new measurements—see Fig. 1. The task is here to identify the distribution labelled as ‘truth’ with ten updates of N samples (where $N = 10, 100, 1000$ was used), and we start with a very broad Gaussian prior (in blue). Here we see the ability of the polynomial based LBU, the PCEKF, to identify highly non-Gaussian distributions, the posterior is shown in red and the pdf estimated from the samples in green; for further details see [25].

The next example is also from [25], where the system is the well-known Lorenz-84 chaotic model, a system of three nonlinear ordinary differential equations operating in the chaotic regime. Remember that this was originally a model to describe the evolution of some amplitudes of a spherical harmonic expansion of variables describing world climate. As the original scaling of the variables has been kept, the time axis in Fig. 2 is in *days*. Every ten days a noisy measurement is performed and the state description is updated. In between the state description evolves according to the chaotic dynamic of the system. One may observe from Fig. 2 how the uncertainty—the width of the distribution as given by the quantile lines—shrinks every time a measurement is performed, and then increases again due to the chaotic and hence noisy dynamics. Of course, we did not really measure world climate, but rather simulated the ‘truth’ as well, i.e. a *virtual* experiment, like the others to follow. More details may be found in [25] and the references therein.

From [30, 31] we take the example shown in Fig. 3, a linear stationary diffusion equation on an L-shaped plane domain as alluded to in Section 1.

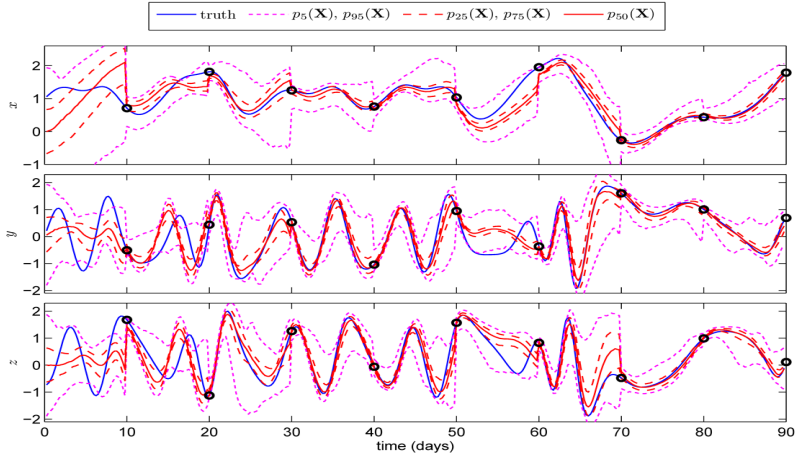


Figure 2: Time evolution of Lorenz-84 state and uncertainty with LBU

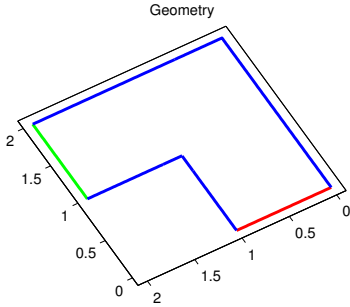


Figure 3: Diffusion domain

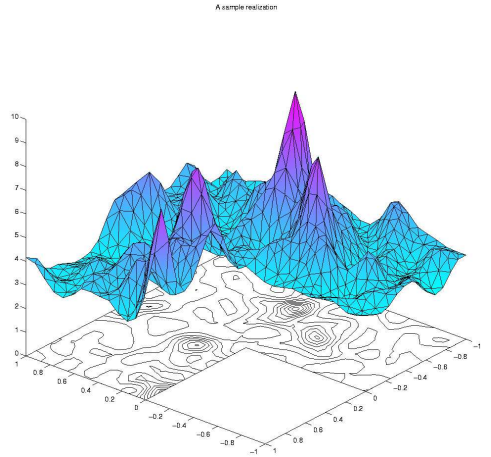


Figure 4: Conductivity field

The diffusion coefficient κ in Eq. (2) is to be identified. As argued in [29], it is better to work with $q = \log \kappa$ as the diffusion coefficient has to be positive, but the results are shown in terms of κ .

One possible realisation of the diffusion coefficient is shown in Fig. 4. More realistically, one should assume that κ is a symmetric positive definite tensor field, unless one knows that the diffusion is *isotropic*. Also in this case

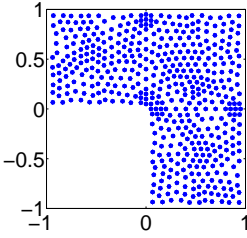


Figure 5: 447 measurement patches

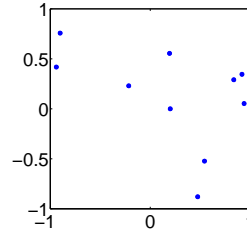


Figure 6: 10 measurement patches

one should do the updating on the logarithm. For the sake of simplicity we stay with the scalar case, as there is no principal novelty in the non-isotropic case.

The virtual experiments use different right-hand-sides f in Eq. (2), and the measurement is the observation of the solution u averaged over little patches, two of these arrangements are shown in Fig. 5 and Fig. 6.

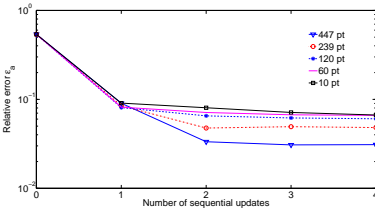


Figure 7: Convergence of identification

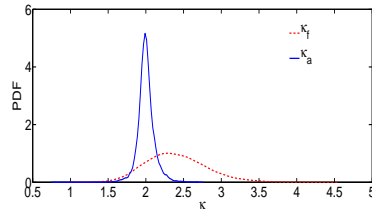


Figure 8: Prior and posterior

In Fig. 7 one may observe the decrease of the error with successive updates, but due to measurement error and insufficient information from just a few patches, the curves level off, leaving some residual uncertainty. The pdfs of the diffusion coefficient at some point in the domain before and after the updating is shown in Fig. 8, the ‘true’ value at that point was $\kappa = 2$. Further details can be found in [30, 31].

As a last example with LBU, we take a strongly nonlinear and also non-smooth situation, namely elasto-plasticity with linear hardening and large deformations and a *Kirchhoff-St. Venant* elastic material law [29, 32]. This example is known as *Cook’s membrane*, and is shown in Fig. 9 with the undeformed mesh (initial), the deformed one obtained by computing with average values of the elasticity and plasticity material constants (deterministic), and finally the average result from a stochastic forward calculation of the probab-

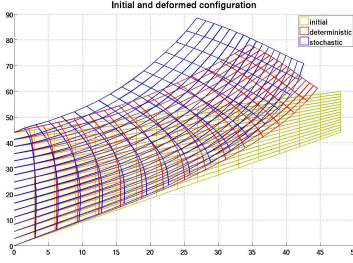


Figure 9: Deformations

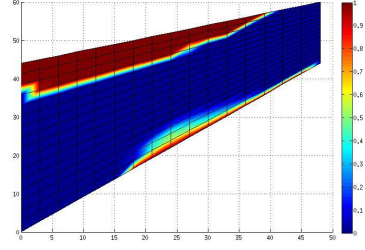


Figure 10: Exceedance probability

ilistic model (stochastic), which is described by a variational inequality [32]. In Fig. 10 one may get another impression of results of the forward model, the probability of the *von Mises* stress being beyond a certain value.

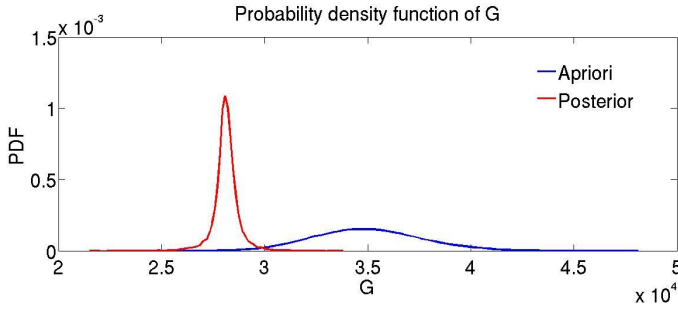


Figure 11: Prior and posterior of shear modulus

The shear modulus G has to be identified, which is made more difficult by the non-smooth nonlinearity. In Fig. 11 one may see the prior and posterior distributions of the shear modulus at one point in the domain. The ‘truth’ is $G \approx 2.7$, and one may observe that the update is successful although the prior density almost vanishes at $G = 2.7$.

5 The nonlinear Bayesian update

In this Section we want to show a computation with the case $n = 2$ of up to quadratic terms in Eq. (14). We go back to the example of the chaotic Lorentz-84 [25] model already shown in Section 4. For this kind of experiment it has several advantages: it has only a three-dimensional state space,

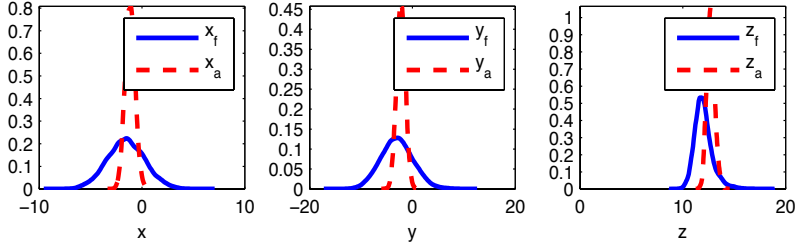


Figure 12: Linear measurement: prior and posterior after one update

these are the uncertain ‘parameters’, i.e. $(x, y, z) \in \mathcal{Q} = \mathbb{R}^3$, the corresponding operator A in the abstract Eq. (1) is sufficiently nonlinear to make the problem difficult, and adding to this we operate the equation in its chaotic regime, so that new uncertainty is added between measurements.

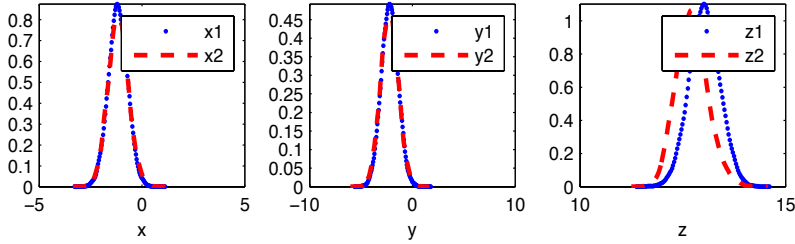


Figure 13: Linear measurement: Comparison posterior for LBU ($n = 1$) and NLBU ($n = 2$) after one update

As a first set of experiments we take the measurement operator to be linear in q ; $Y(q) = q = (x, y, z)$, i.e. we can observe the *whole* state directly. At the moment we consider updates after each day—whereas in Fig. 2 the updates were performed every 10 days. The results for the pdfs of the state variables are shown in Fig. 12, where the prior and the posterior pdf for a LBU after one update are given. Then we do the same experiment, but with a *quadratic* nonlinear BU (NLBU) with $n = 2$. The results for the posterior pdfs are given in Fig. 13, where the linear update is dotted in blue, and the full red line is the quadratic NLBU; there is hardly any difference between the two. This might have been expected after our discussion at the end of Subsection 2.3. If we go on to the second update—after two days—some differences appear, the results for the posterior pdfs are in Fig. 14.

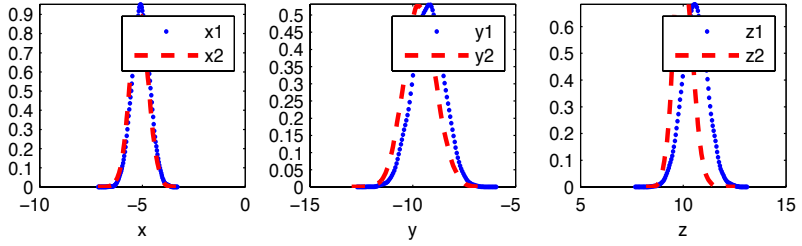


Figure 14: Linear measurement: Comparison posterior for LBU ($n = 1$) and NLBU ($n = 2$) after second update

As the differences between LBU and NLBU with $n = 2$ were small—we take this as an indication that the LBU is not too inaccurate an approximation to the conditional expectation—we change the experiment and take a nonlinear measurement function, which is now cubic: $Y(q) = (x^3, y^3, z^3)$. As discussed at the end of Subsection 2.3, we now expect larger differences between LBU and NLBU.

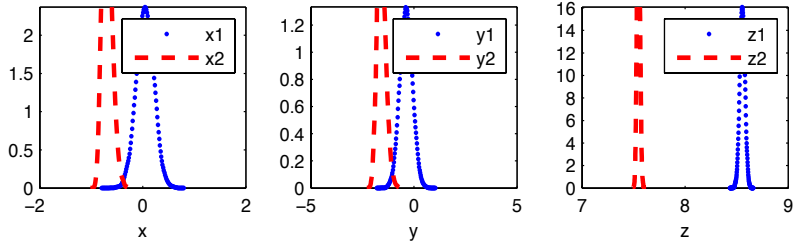


Figure 15: Cubic measurement: Comparison posterior for LBU ($n = 1$) and NLBU ($n = 2$) after one update

These differences in posterior pdfs after one update may be gleaned from Fig. 15, and they are indeed larger than in the linear case Fig. 13, due to the strongly nonlinear measurement operator.

As the cubic is quite a strong nonlinearity, we performed a set of experiments where the measurement function is $Y(q) = (x|x|, y|y|, z|z|)$; only a quadratic nonlinearity, but no loss of information about the sign like in the small example at the end of Subsection 2.3. The updates are performed every day, the Fig. 16, which shows the trajectory of one state variable, corresponds in that way to Fig. 2.

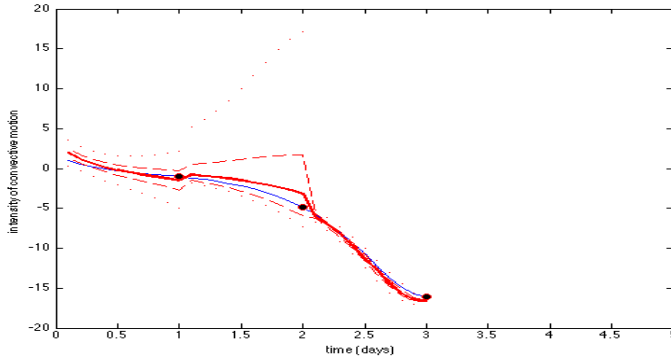


Figure 16: Partial state trajectory with uncertainty and three updates

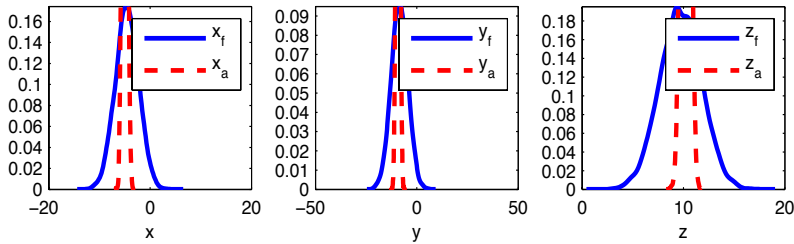


Figure 17: Quadratic measurement: Comparison posterior for LBU ($n = 1$) and NLBU ($n = 2$) after one update

The results for the 2-nd update are displayed for the posterior pdfs in Fig. 17. This has to be compared Fig. 14, and the differences are indeed much larger.

6 Conclusion

Here we have tried to show the connection between inverse problems and uncertainty quantification. An abstract model of a system was introduced, together with a measurement operator, which provides a possibility to predict—in a probabilistic sense—a measurement. The framework chosen is that of Bayesian analysis, where uncertain quantities are modelled as random variables. New information leads to an update of the probabilistic description

via Bayes's rule.

After elaborating on the—often not well-known—connection between conditional probabilities as in Bayes's rule and conditional expectation, we set out to compute and—necessarily—approximate the conditional expectation. As a polynomial approximation as chosen, there is the choice up to which degree one should go. The case with up to linear terms—the linear Bayesian update—is best known and intimately connected with the well-known Kalman filter. In addition, we show how to compute approximations of higher order.

There are several possibilities on how one may choose a numerical realisation of these theoretical concepts, and we decided on functional or spectral approximations. It turns out that this approach goes very well with recent very efficient approximation methods building on separated or so-called low-rank tensor approximations.

Starting with the linear Bayesian update, we show a series of examples of increasing complexity. The method works well in all cases. One of the examples is then chosen to show the nonlinear Bayesian update, where we go up to quadratic terms. A series of experiments is chosen with different measurement operators, which have quite a marked influence on whether the linear and quadratic update are close to each other.

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